An empirically constructed dynamic electric dipole polarizability function of magnesium and its applications

James F. Babb

Harvard-Smithsonian Center for Astrophysics, 60 Garden St., MS 14, Cambridge, MA 02138

(Dated: August 28, 2015)

The dynamic electric dipole polarizability function for the magnesium atom is formed by assembling the atomic electric dipole oscillator strength distribution from combinations of theoretical and experimental data for resonance oscillator strengths and for photoionization cross sections of valence and inner shell electrons. Consistency with the oscillator strength (Thomas-Reiche-Kuhn) sum rule requires the adopted principal resonance line oscillator strength to be several percent lower than the values given in two critical tabulations, though the value adopted is consistent with a number of theoretical determinations. The static polarizability is evaluated. Comparing the resulting dynamic polarizability as a function of photon energy with more elaborate calculations reveals the contributions of inner shell electron excitations. The present results are applied to calculate the long-range interactions between two and three magnesium atoms and the interaction between a magnesium atom and a perfectly conducting metallic plate. Extensive comparisons of prior results for the principal resonance line oscillator strength, for the static polarizability, and for the van der Waals coefficient are given in an Appendix.

PACS numbers: 34.20.Cf, 32.10.Dk, 31.10.+z

I. INTRODUCTION

Magnesium is an abundant element currently of interest in several applications. Analysis of photo association spectroscopy for the Mg dimer [1, 2] indicates that the s-wave scattering length for collisions between two ground state Mg atoms is positive [1], with the accuracy of the determination affected by the remnant uncertainty in the value of the atom-atom van der Waals constant [2]. (A Bose-Einstein condensate of Mg atoms has not been created experimentally, to date.) However, a determination of the leading term in the long-range interaction of electronically excited states of the Mg dimer, which is related to the principal resonance line oscillator strength, using molecular spectroscopy has been elusive [3]. Mg atoms were investigated as a possible sympathetic cooling agent in collisions with NH [4, 5] and Lonij *et al.* [6] theoretically explored the interaction of an Mg atom with a wall for applications to atom interferometry. And, while Mg is abundant in the solar system, it is interesting to note that the Mg principal resonance line was recently detected in the observation of the exoplanet HD 209458b using transit spectroscopy [7]. Modeling Mg absorption in exoplanet atmospheres depends proportionally on the principal resonance line absorption oscillator strength [8], the value of which in turn affects the use of that line as a probe of escaping atoms in exoplanet atmospheric spectroscopy [9].

An analysis of the dynamic electric dipole polarizability function of Mg is valuable for several reasons. First, because the principal resonance line oscillator strength is an important contributor to the function, it is possible to determine a value that achieves consistency with oscillator strength sum rules. Secondly, it is desirable to have an independent assessment of the completeness of existing elaborate calculations of the function itself, for which extensive tabulations from two different types of calculations are available [10, 11].

Calculations of dynamic electric dipole polarizabilities are of intrinsic theoretical interest due to the challenges inherent in treating correlations and excitations of all electrons quantum-mechanically at different photon energies [12, 13]. Such calculations are necessarily important benchmarks for theoretical methods applied to photoabsorption [14], photodetachment [15], blackbody radiation shifts [16–18] and AC Stark shifts [19], magic wavelengths [20], and parity non conservation amplitudes [21], as well as being helpful in the ongoing development of density functional theory (DFT) methods for dispersion forces (cf. [22–26]). In addition, for metals experimental data at a wide spectrum of photon energies are relatively scarce though X-ray data, and sometimes optical data [27, 28], are available. There is recent progress for systematically measuring static polarizabilities [29]. Many theoretical approaches are available, but their reliability in calculating dynamic polarizabilities can be difficult to gauge without critical evaluation, but critical evaluations are limited to the static polarizabilities [30–32]. Nevertheless, dynamic polarizabilities are of great utility in calculating coefficients appearing in certain potential energies, particularly van der Waals constants (for investigations of ultra-cold collisions, for photo association spectroscopy, and for ultra-cold gas studies) and Lennard-Jones constants (for atom-surface interactions, where recent applications include tests for gravity-related new physics at submillimeter distances [33–35], optical clocks [36, 37], atom-graphene interactions [38], noncontact van der Waals friction [39], and interactions between nanostructures [40]).

In a previous paper treating the sodium atom [41], a semi-empirical theory utilizing oscillator strength sum rules and input data from experiments and calculations predicted a value of the van der Waals coefficient [41], which was found to be in harmony with subsequent experimentally determined fits from photo-association spectroscopy data [42, 43] and *ab initio* theoretical methods [44]. In the case of sodium, the availability of precise measurements of the principal resonance line oscillator strength from photo-association spectroscopy and of the static electric dipole polarizability from atom interferometry augmented the semi-empirical analysis [41]. In the case of magnesium, such data are not available. Therefore, in this paper, for Mg, the electric dipole oscillator strength distribution is composed using extant data on electric dipole oscillator strengths, photoabsorption cross sections, and energies obtained experimentally and theoretically. As will be shown, consistency with the oscillator strength (Thomas-Reiche-Kuhn) sum rule requires a value of the principal resonance line oscillator strength that is several percent lower than values listed in critical tabulations by Morton [45] and by Kelleher and Podobedova [46]. Other evidence for the value adopted is given. The static electric dipole polarizability is evaluated and compared with other values. The dynamic polarizability function is calculated and compared with previous results obtained by Porsev et al. [10] using configuration interaction and many-body perturbation theory with core contributions (CI-MBPT) [47] and by Jiang *at al.* [11] using the configuration interaction with semi-empirical core-valence interaction (CICP) method. The present dynamic polarizability function is used to evaluate the van der Waals constant, Axilrod-Teller-Muto constant, and atom-surface interactions. Results from the literature for the principal resonance line oscillator strength, static electric dipole polarizability, and van der Waals constant are collected and compared in the Appendix.

II. DIPOLE OSCILLATOR STRENGTH SUM RULES

The absorption oscillator strength from the ground state $|0\rangle$ with eigenvalue E_0 to an excited state $|n\rangle$ with eigenvalue E_n is

$$f_n = \tfrac{2}{3}(E_n - E_0)\left|\left\langle 0 \left|\sum_{i=1}^{N}\mathbf{r}_i\right| n \right\rangle\right|^2, \tag{1}$$

where $\mathbf{r}_i$ is the position vector of electron i, and N is the number of electrons. Atomic units are used throughout unless otherwise specified.

Denoting by S'_n the sum-integral (the sum over all discrete transitions excluding the initial state and the integration over all continuum states), the resultant sum rules are

$$S(0) = \mathsf{S}'_n f_n = N, \tag{2}$$

with $N = 12$ for Mg,

$$S(-1) = \mathsf{S}'_n f_n/(E_n - E_0) = \tfrac{2}{3} \left\langle 0 \left| \left(\sum_{i=1}^N \mathbf{r}_i \right)^2 \right| 0 \right\rangle, \tag{3}$$

and

$$S(-2) = \mathsf{S}'_n f_n/(E_n - E_0)^2 = \alpha(0), \tag{4}$$

where $\alpha(0)$ is the static electric dipole polarizability. The dynamic electric dipole polarizability function is

$$\alpha(\omega) = \mathsf{S}'_n \frac{f_n}{(E_n - E_0)^2 - \omega^2}, \tag{5}$$

where ω is the photon energy. By direct integration the $S(-1)$ sum rule is related to the atom-wall interaction coefficient C_3 [41]

$$C_3 = \tfrac{1}{8} S(-1) = \frac{1}{4\pi} \int_0^\infty d\omega \, \alpha(i\omega), \tag{6}$$

the van der Waals coefficient is

$$C_6 = \frac{3}{\pi} \int_0^\infty d\omega \, [\alpha(i\omega)]^2, \tag{7}$$

and the Axilrod-Teller-Muto coefficient is

$$C_9 = \frac{3}{\pi} \int_0^\infty d\omega \, [\alpha(i\omega)]^3. \tag{8}$$

III. OSCILLATOR STRENGTH DISTRIBUTION

A magnesium atom has twelve electrons. Their configuration is $(1s^2 2s^2 2p^6 3s^2)\ {}^1S_0$.

A. Discrete transitions

Sources with tabulations of values, experimental and theoretical, for the absorption oscillator strengths are Mitchell [48], Mendoza and Zeippen [49], Ray and Mukherjee [50], Jönsson and Fischer [51], Hamonou and Hibbert [52], and Derevianko and Porsev [53].

There are numerous theoretical determinations of the oscillator strength for the principal resonance line $(3s^2)\ {}^1S - (3s3p)\ {}^1P^o$. A detailed survey is given in the Appendix. Reliable theoretical calculations range from 1.709 to 1.76, and there were at least ten experimental determinations as of 2003 [45]. In a critical review, Morton [45] adopted a value of 1.83 ± 0.03 based on a weighted mean of the ten experimental values. A long-standing discrepancy between

experimental and theoretical trends was noted previously [54–57]. The tendency of high-level theoretical results to be less than 1.8 was noted recently by Zatsariny *et al.* [57] who calculated a nonrelativistic value of 1.738 and pointed out that a "very extensive and essentially converged multiconfiguration Hartree-Fock (MCHF)" *ab initio* calculation by Jönsson, Fischer, and Godefroid [56] found 1.717. Jönsson, Fishcher, and Godefroid [56], using the observed transition energy to evaluate the oscillator strength, obtained 1.710 and also pointed out (see their Table 11) that (as of 1999) theoretical values were consistently smaller than the experimental ones (to date) by about 5 percent. Recently, Derevianko and Porsev [53] quote for the matrix element governing the line strength a value 4.03 ± 0.02 with error of 0.5% based on their calculations from 2001 [58]; the corresponding oscillator strength using the experimental transition energy [46] is 1.73 ± 0.02. The original NIST (NBS) tabulation of 1969 [59] adopts 1.8 ± 0.18 from an average of the experiments of Refs. [60, 61] and the calculation of Weiss [62]. The value 1.8 (cited as a private communication from A. W. Weiss) is given with 3 percent error (± 0.05) at the 90 percent confidence level in the 2008 NIST revised tabulation [46].

I adopt the value 1.75, which is the lower limit of the value 1.80(5) from Kelleher and Podobedova [46] and the upper limit of the value 1.73(2) recommended by Derevianko and Porsev.

Mitchell [48] used the anomalous dispersion (hook) method to measure the second ($3s$–$4p$) through sixth ($3s$–$8p$) resonance transition oscillator strengths and found, respectively, 0.107 ± 0.0019, $(2.27 \pm 0.12) \times 10^{-2}$, $(8.53 \pm 0.46) \times 10^{-3}$, $(4.11 \pm 0.36) \times 10^{-3}$, and $(2.34 \pm 0.15) \times 10^{-3}$, all determined relative to the value of 1.72 for the principal transition that Victor and Laughlin [63] calculated using a semi-empirical model potential method. Other theoretical determinations of f values for the second and higher resonance transitions are those of Saraph [64], Mendoza and Zeippen [49], Chang and Tang [65] and Zatsarinny *et al.* [57]. I adopt the values of Chang and Tang, who calculated for the principal to sixth resonance lines, respectively, oscillator strengths 1.75, 0.111, 0.024, 0.0091, 0.0043, and 0.0024. These five discrete (second to sixth resonance) transitions contribute 0.151 to the $S(0)$ sum and 2.81 to the $S(-2)$ sum for the $3s$ shell.

Including the principal resonance line, the *discrete transition* contribution from the $3s$ shell to $S(0)$ is 1.90 and to $S(-2)$ is 71.4.

B. Continuum transitions

A number of sources exist for the continuum oscillator strengths corresponding to the ejection of a $3s$ electron [66–86]. The photoionization cross sections calculated using a variational MCHF method by Fischer and Saha [74] are in good agreement with the experimental results of Wehlitz *et al.* [82]. The threshold cross section of 2.5 Mb calculated by Fischer and Saha [74] is slightly larger than both the value 2.1 ± 0.3 Mb measured by Fung *et al.* [80] and the value 2.36 ± 0.02 Mb that Parkinson, Reeves, and Tomkins [69] found by extrapolation from the measured discrete oscillator strengths of Ref. [48]. Wehlitz *et al.* [82] normalized their own measurements to the value 2.1 Mb at threshold. At a photon energy of 30 eV, a recent calculation by Pindzola *et al.* [85] using a time-dependent close-coupling method with an effective core potential gives $\sigma_{3s}(30\,\text{eV}) = 0.217$ Mb, while Verner *et al.* [78] calculate 0.255 Mb. At 80 eV, the "complete" experiment of Haussman *et al.* [83], for which the total absorption cross section of Ref. [87] was used for normalization, yields $\sigma_{3s}(80\,\text{eV}) = 0.080 \pm 0.011$ Mb from the main transition compared to the value 0.087 from Verner *et al.* Haussman *et al.* also measured an additional 0.014 ± 0.004 Mb contribution from satellites. The measurements of Wehlitz *et al.* [82] are adopted for energies from threshold to 11.6 eV and the $3s$ cross section data were extended to higher energies using the results of Verner *et al.* [78].

The contributions to the three sum rules $S(0)$, $S(-1)$, and $S(-2)$ from the continuum are, respectively, 0.261, 0.162, and 0.277. Combining these with the discrete contributions from the Sec. III A the total valence shell contributions are 2.16, 11.8, and 71.7, which are listed in Table I. The calculated valence shell contribution of 2.16 to the $S(0)$ sum confirms that the contribution from the $3s$ electron to $S(0)$ is greater than 2 [88, 89], indicating configuration interaction of the valence electrons with the core electrons. Maeder and Kutzelnig [90] obtained 2.06 using a model potential including core-valence correlation.

The excitation and ejection of K shell electrons was considered by Verner *et al.* [78], Kutzner *et al.* [91], and Hasoğlu *et al.* [92]. Hasoğlu *et al.* used R-matrix methods to calculate excitation of K shell electrons to np states resonant below the threshold. The resonances are estimated to contribute 0.03 to the value of $S(0)$. The relativistic random-phase approximation modified to include relaxation effects (RRPAR) calculations of Kutzner *et al.* are in good agreement with the cross sections calculated by Verner *et al.* from threshold to high energies. Banna *et al.* [93] measured the shake-up peak just above the threshold, but absolute cross sections are not available. The cross sections of Verner are adopted from the threshold for ejection of a $1s$ electron at 1310.9 eV. The K shell contribution yields 1.56 to $S(0)$ and it is negligible for $S(-1)$ and $S(-2)$. The $1s$ contribution to $S(0)$ found here for Mg is comparable to that found for Na [41].

Deshmukh and Manson [70], Nasreen, Manson, and Deshmukh [94], Kutzner *et al.* [91], and Verner *et al.* [78] calculated the partial cross sections for the ejection of a $2s$ electron. The cross section value 0.3 Mb at the threshold energy of 94.0 eV is adopted [91, 94] and linearly joined to the results of Verner *et al.* at 270 eV, which are used for higher energies. For the $2s$ shell the contribution to the sums $S(0)$, $S(-1)$, and $S(-2)$ are, respectively, 1.02, 0.1, and 0.02.

The remaining oscillator strength must come from the $2p$ shell and the expected contribution to $S(0)$ is 7.26.

Deshmukh and Manson [70], Altun [77], Nasreen, Manson, and Deshmukh [94], Kutzner, Maycock, and Thorarinson [91], investigated photoionization of a $2p$ electron. There a number of resonances corresponding to excitation to autoionizing states [77] and they contribute significantly to the oscillator strength. Measurements of the cross section by Haussman *et al.* [83] at 80 eV found that the resonances constitute 25% of the $2p$ shell photoionization cross section. The cross sections averaged over the resonances from the correlated length gauge many-body perturbation theory (MBPT) calculations of Altun (Figure 9 of Ref. [77]) are adopted from 63.29 eV to 344.89 eV, giving $\sigma_{2p}(80\,\text{eV})$ = 6.2 Mb which is slightly larger than the reference value used by Haussman *et al.* The calculations of Verner *et al.* are used from the threshold energy of 54.9 eV up to 63.29 eV and for energies above 344.89 eV. These data yield for the $2p$ shell the contributions to the sums $S(0)$, $S(-1)$, and $S(-2)$, respectively, 7.33. 1.61, and 0.45. If the calculations of Altun are multiplied by a factor of 0.985, the cross section at 80 eV becomes 6.1 Mb and the sums $S(0)$, $S(-1)$, and $S(-2)$ are calculated to be, respectively, 7.26, 1.60, and 0.44 and the values are listed in Table I.

The contributions to the sums $S(0)$, $S(-1)$, and $S(-2)$ from the excitation of the $1s$, $2s$, $2p$, and $3s$ electrons are summarized in Table I.

C. Discussion

Stwalley [88], Pal'chikov and Ovsiannikov [95], Ovsiannikov *et al.* [96], and Sarkisov *et al.* [28] constructed oscillator strength distributions of Mg for calculations of dynamic polarizabilities, considering valence transitions. Sarkisov *et al.* [28] included an estimate of $2p$ excitations.

From their tabulated data, the results of Pal'chikov and Ovsiannikov [95] and Ovsiannikov *et al.* [96] indicate a total

TABLE I: Contributions to the sum rule $S(k)$ for Mg.

	$S(0)$	$S(-1)$	$S(-2)$
1s	1.56	0.02	...
2s	1.02	0.10	0.02
2p	7.26	1.60	0.44
3s	2.16	11.8	71.7
Total	12.0	13.5	72.2

discrete contribution of 1.9 to the $S(0)$ sum rule for $3s$ discrete transitions in agreement with the present result. They used a value of 1.73 for the principal resonance line oscillator strength, which offsets in the sum rule their slightly larger value of 0.122 for the second resonance line oscillator strength, compared to the present adopted values of, respectively, 1.75 and 0.111. For the $S(-2)$ sum, they find for the second to sixth resonance transitions a contribution of 3.12 to $S(-2)$, to be compared to the present value of 2.81. The difference between their value and the present value is due primarily to the different values of the second resonance line oscillator strength. Their total value (valence electrons) for $S(-2)$ is 71.39, while the present value for the $3s$ shell is 71.7.

Including all shells, the present value of $\alpha(0)$ is 72.2 from the $S(-2)$ sum rule, see Table I. It lies only 0.2 above the range of values 71.3(7) recommended by Porsev and Derevianko [47] and it is compared with a number of other theoretical calculations in the Appendix.

Note that if the value 1.8 is adopted for the principal oscillator strength [46], without any other adjustments to the adopted data, the present $S(0)$ sum becomes 12.05 and $\alpha(0)$ becomes 73.4, which is far beyond the value recommended by Porsev and Derevianko. The value 1.83 for the oscillator strength adopted by Morton [45] is more difficult to reconcile within the present analysis. The $S(0)$ sum becomes 12.08 and the value of $\alpha(0)$ becomes 74.6. Sarkisov *et al.* [28] use the oscillator strength data from Morton [45] and estimate the $2p$ and $3s$ continuum contributions using the data from Verner *et al.* [78] and find $\alpha(0) = 73.6$. Stwalley's early calculation [88] used the value 1.82(5) for the principal resonance line oscillator strength (see his Ref. 7 for sources) and obtained an estimate $\alpha(0) = 75.0 \pm 3.0$.

A recent experiment [29] using a pulsed cryogenic molecular beam electric deflection method obtained a value $\alpha(0) = 59(15)$, which is not sufficiently accurate to discriminate between theoretical calculations.

Reshetnikov *et al.* [89] explored the relationship between the uncertainty in $\alpha(0)$ and the uncertainty in the lifetime of the first resonance transition in two-valence electron atoms and ions. Their formalism allows a valence shell contribution to N that is not exactly 2, as found here and in Ref. [90]. In terms of the the valence contribution, N_e, the principal resonance line oscillator strength $f_{3s,3p}$, and the excitation energies of the first and second resonance transitions, respectively, $E_{3s,3p}$ and $E_{3s,4p}$, they give

$$\alpha(0) = \frac{f_{3s,3p}}{E_{3s,3p}^2} + \frac{N_e - f_{3s,3p}}{2E_{3s,4p}^2} \tag{9}$$

and an uncertainty estimate for the polarizability

$$\Delta\alpha(0) = \frac{N_e - f_{3s,3p}}{2E_{3s,4p}^2}. \tag{10}$$

Using the present adopted value $f_{3s,3p} = 1.75$, calculated value $N_e = 2.16$, and transition energies [46] $E_{3s,3p} = 0.159\,705$ and $E_{3s,4p} = 0.224\,840$, yields an estimate $\alpha(0) = 72.7 \pm 4$. Likewise, using their formula for estimating the uncertainty of $f_{3s,3p}$, given the present calculated value $\alpha(0) = 72.2$, yields $f_{3s,3p} = 1.79 \pm 0.07$. The formulae of
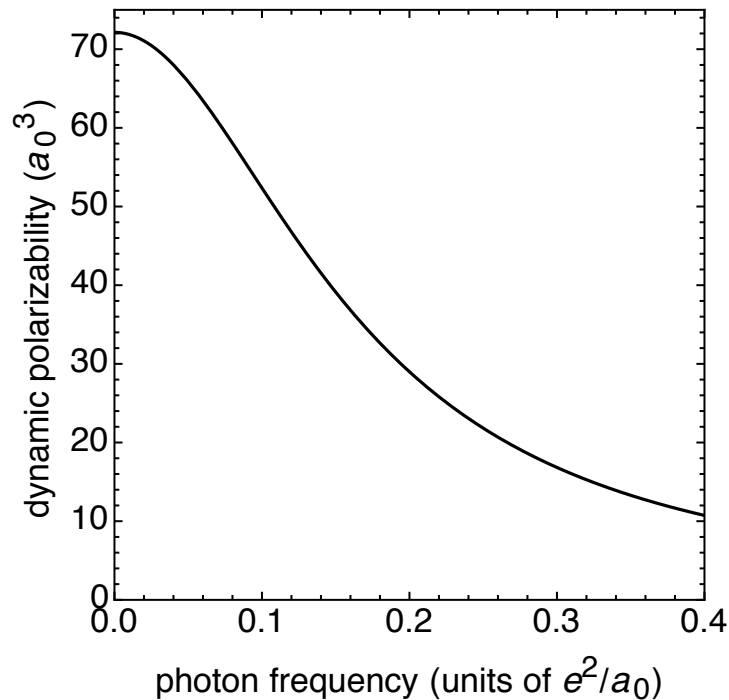
FIG. 1: The dynamic dipole polarizability function $\alpha(i\omega)$ from the present calculations.

Reshetnikov *et al.* [89] demonstrate that the present results are mutually consistent, but the estimates obtained are not sufficiently precise to allow selection of a particular value of $f_{3s,3p}$ from the many available values, see Appendix.

The availability of a more accurate measurement of $\alpha(0)$ and a definitive measurement of the principal resonance line lifetime would significantly improve the present model [41]. Nevertheless, the values adopted here, in particular $f_{3s,3p} = 1.75$, generate sum rules that are consistent and not in contradiction with other major studies, while a value of $f_{3s,3p} \geq 1.8$ is inconsistent.

IV. DYNAMIC ELECTRIC DIPOLE POLARIZABILITY FUNCTION

The dynamic electric dipole polarizability function at imaginary frequencies is constructed using the discrete and continuum oscillator strength data as assembled in Sec. III.

The continuum oscillator strength distribution is given in terms of the photoionization cross section $\sigma(E)$ by

$$\frac{df}{dE} = \frac{\sigma(E)}{2\pi^2 \alpha_{\mathrm{fs}}}, \quad E > 0.281, \tag{11}$$

with α_{fs} the fine structure constant, and the dynamic dipole polarizability at imaginary energy is

$$\alpha(i\omega) = \sum_n \frac{f_n}{(E_n - E_0)^2 + \omega^2} + \int dE \, \frac{df/dE}{E^2 + \omega^2}. \tag{12}$$

The function $\alpha(i\omega)$ resulting from the analysis in Sec. III is shown at low energies in Fig. 1. It may be compared with the calculations of Derevianko *et al.* [10] and those of Jiang *et al* [11]. The present function $\alpha(i\omega)$ was evaluated at the fifty energies corresponding to the energies ω_k of a 50-point quadrature, as listed in Table A of Ref. [10], and the energies for a 40-point quadrature listed in Table C of Jiang *et al.* In Fig. 2 the data are plotted. Agreement is very good between the present results and the CI-MBPT results of Ref. [10]. There are noticeable discrepancies
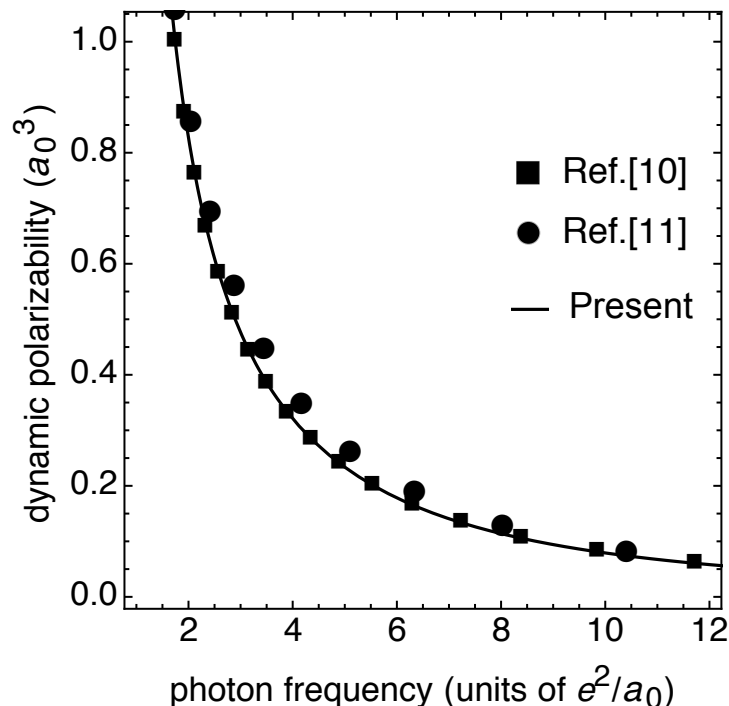
FIG. 2: For the dynamic dipole polarizability function $\alpha(i\omega)$, comparison between the present values (line), the configuration interaction with semi-empirical core-valence interaction (CICP) values from Ref. [11] (circles), and the configuration interaction and many-body perturbation theory with core interactions (CI-MBPT) values from Ref. [10] (squares).

between the present results and the CICP results of Ref. [11]. To further investigate the discrepancies, in Fig. 3 the percentage difference between the values from the functions given in Ref. [10] or Ref. [11] and the present values are shown. The present model and the calculations of Ref. [10] agree within several percent at all energies. The present values are larger than those of Ref. [10] at low energies, due to the larger principal oscillator strength adopted herein. The several percent agreement across all energies is satisfactory and a more detailed analysis might await an accurate experimental value for $\alpha(0)$ and a definitive measurement of the principal resonance line oscillator strength. In contrast, the differences between the present model and the model of Ref. [11] are made apparent in Fig. 3 showing that the CICP model of Ref. [11] yields larger values for $\alpha(i\omega)$ in the energy range of 1 to 200 au. The difference may arise due to the choice of "effective" core oscillator strengths in the CICP model [11, 97]. The percent difference peaks at about 16 % around 5–6 e^2/a_0 (135–160 eV) placing the missing oscillator strength of the CICP model in the inner s shells, where the "effective" oscillator strengths are placed to model inner shell absorption [11, 97].

V.   APPLICATIONS

A.   van der Waals coefficient C_6

The long-range potential energy between two Mg atoms separated by a distance R is $-C_6/R^6$, where C_6 is given by Eq. (7). For the van der Waals coefficient, I find $C_6 = 642.4$ by evaluating Eq. (7) using the quadrature method
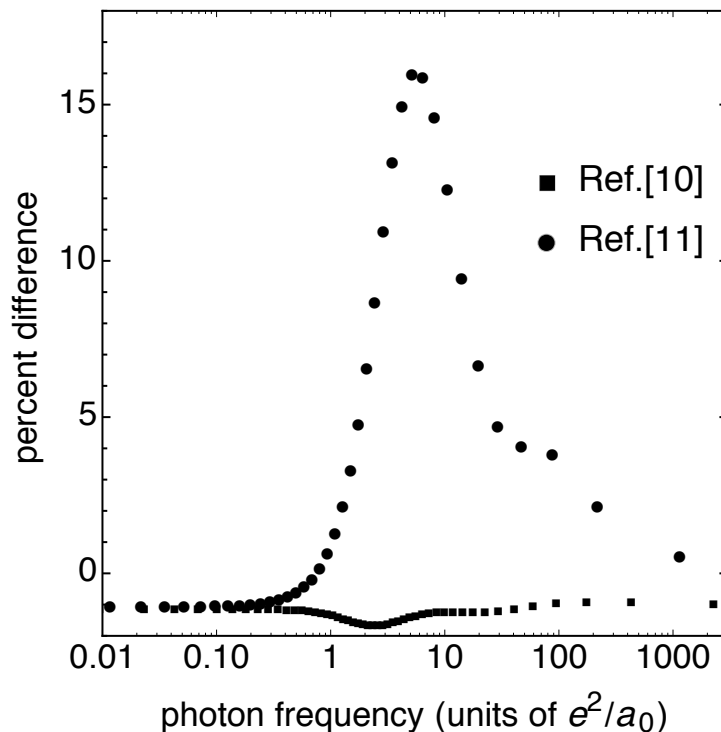
FIG. 3: For the dynamic dipole polarizability function $\alpha(i\omega)$, percent difference comparison between the present values and the CI-MBPT values from Ref. [10] and between the CICP values from Ref. [11] . The quantity plotted is $100 \times [(\text{other}) - (\text{present})]/\text{present}$, where "other" is either Ref. [10] or [11]. The filled squares are the percent differences of the present values from the CI-MBPT values and the filled circles are the percent differences of the present values from the CICP values. The plotted values show that the present $\alpha(i\omega)$ is within several percent of the CI-MBPT values across the range of energies and show that the CICP values are larger for photon energies between roughly 1 and 200 atomic units.

of Ref. [10],

$$C_6 \approx \frac{3}{\pi} \sum_{j=1}^{50} w_j \alpha^2(i\omega_j), \tag{13}$$

using the present values of $\alpha(i\omega)$ evaluated at the energies ω_j and with the weights w_j given in Table A of Ref. [10]. Porsev and Dereveanko [98] quote accuracy of 2% or better for their value $C_6 = 627(12)$ obtained using a semi-empirical hybrid relativistic many-body perturbation theory (CI-MBPT) approach. The present value lies just above their range, mainly corresponding to their principal resonance line oscillator strength of 1.73, compared to the present adopted value of 1.75, thus, $642 \times (1.73/1.75)^2 \approx 627$. The present result improves upon the earlier empirical estimate of 683(35) by Stwalley [88]. A more detailed survey and comparison of other determinations of C_6 is given in the Appendix.

B.   Atom-wall coefficient C_3

The long-range potential energy of an Mg atom at distance z from a perfectly conducting wall is $-C_3/z^3$, where C_3 is given by Eq. (6). Mitroy and Bromley [97] calculated $C_3 = 1.704$ using the CICP approach, while the CI-MBPT value is 1.666 [10]. Lonij et al. [6] gave an approximate value of 1.51 using a limited 4-parameter model for the

dynamic polarizability. The value of C_3 is known to be sensitive to the completeness of the description of the core electrons [44, 99, 100].

The present value is $C_3 = 1.69$ using $C_3 = \frac{1}{8}S(-1)$ and the value of $S(-1)$ from Table I and 1.687 using Eq. (6) and the quadrature from Ref. [10],

$$C_3 \approx \frac{1}{4\pi} \sum_{j=1}^{50} w_j \alpha(i\omega_j). \tag{14}$$

Both of the present values (sum rule and quadrature) are in larger than that of Ref. [10]. The slightly larger value of C_3 from the CICP calculations, Ref. [11], is consistent with the relatively larger values of $\alpha(i\omega)$, as discussed in Sec. IV and shown in Figs. 2 and 3.

C. Other properties

The Axilrod-Teller-Muto coefficient C_9, Eq. (8), characterizes the mutual long-range interaction potential of three atoms. The value obtained by Mitroy and Bromley [97] is $33\,380$ and that obtained by Porsev *et al.* [10] is $33\,241$. Using the dynamic polarizability function I evaluated, Eq. (8), using the quadrature of Ref. [10],

$$C_9 \approx \frac{3}{\pi} \sum_{j=1}^{50} w_j \alpha^3(i\omega_j), \tag{15}$$

and obtained $C_9 = 34\,480$.

The larger value for C_9 found here mainly reflects the larger principal oscillator strength 1.75 adopted compared to the principal oscillator strengths found in Refs. [97] and [10]. The oscillator strength appears as a cubic power in Eq. (15) through $\alpha(i\omega)$, see Eq. (12). For example, comparing to Ref. [10], which used a principal oscillator strength of 1.73, scaling the present value I obtain $34\,450 \times (1.73/1.75)^3 = 33\,310$, which is within 0.2 % of the value of Ref. [10].

VI. CONCLUSION

Experimental and theoretical data were assembled and used to formulate the dynamic polarizability function for Mg. I find that consistency in the sum rules can be achieved using the adopted value of the principal resonance line oscillator strength to be 1.75; lower than the curated values of 1.83 [45] and 1.8 [46], but in agreement with theoretical calculations. Comparisons of the dynamic dipole polarizability functions from the present work and those calculated using the CI-MBPT approach and the CICP approach were presented. Good agreement (within several percent) was found with the CI-MBPT results over all photon energies providing an independent confirmation of the CI-MPBT approach for Mg [10]. For the CICP method the differences were more pronounced, approaching 16% at energies around 5–6 e^2/a_0, or about 135–160 eV, indicating that the "effective" oscillator strengths of Refs. [97] and [11] may not completely model oscillator strengths corresponding to the core electrons. To improve the present model it would be valuable to have more accurate experimental measurements of the polarizability and a definitive measurement of the principal oscillator strength. Where sufficient and reliable data is available, the present methodology can be applied to other atoms. *Note added in proof: A recent calculation [Y. Singh, B. K. Sahoo, and B. P. Das, Phys. Rev. A **88**, 062504 (2013)], using a relativistic coupled cluster theory with all singly and doubly excited configurations, found a polarizability value of 72.54(50). I thank Dr. Singh for communicating this result.*

Acknowledgments

Appendix: Values from the literature

In this Appendix, values for Mg of the principal resonance transition oscillator strength, of the static electric dipole polarizability, and of the van der Waals constant are collected from the literature. Some earlier collections include Refs. [48–50, 76] for the principal oscillator strength, Refs. [32, 50, 52, 90, 97, 101] for the polarizability, and Ref. [97] for the van der Waals constant.

For the oscillator strength, as discussed in the Sec. III, it was noted in several recent papers [56, 57] that in general the most sophisticated theoretical calculations lie several percent below the published experimental values, see also earlier similar comments in Refs. [63], [55], and [49]. Also, it was noted that the "best" calculations lie below [57] the adopted value of 1.8 in the NIST tabulation [46]. As shown in Table II, the configuration interaction (CI), multi-configuration Dirac-Fock (MCDF), and multi-configuration Hartree-Fock with Breit-Pauli interactions (MCHF+BP) calculations, are all in general agreement; the latter two methods include relativistic effects. In addition, the semi-empirical model potential (MP) calculation of Victor and Laughlin [63] agrees with the MCHF calculation. In the Table, where treatment of core-valence correlation was included the suffix CV is appended. In addition, the relativistic configuration interaction with the Breit interaction (RCI+Breit) of Ref. [103] are in close agreement with the configuration interaction Dirac-Fock with core polarization (CIDF-CP) calculation of Ref. [104]. CI+MBPT methods use complete relativistic CI calculations for the valence electrons in a frozen core combined with MBPT to account for core-valence interactions. The CI frozen core calculations of Saraph [64] and Chang and Tang [65] and the CI-CV calculations of Moccia and Spizzo [76] are in close agreement with values between 1.75 and 1.76. There is substantial theoretical evidence for a value of the principal oscillator strength around 1.75.

Many calculations of the static polarizability $\alpha(0)$ are available. There are several good tables containing summaries of other earlier works. In particular, from 1976, Reinsch and Meyer [101] and from 1991, Archibong and Thakkar [108], see also Schwerdtfeger [30]. Thakkar and Lupinetti [31] recommend a theoretical value of 71.22 ± 0.36, which includes a relativistic correction of -0.35, and Chu and Dalgarno [109] recommend 71.

Table III lists some of the results from the literature. The quantum defect theory (QDT) value from Chernov *et al.* [110] models the response of the valence electrons only. The pseudopotential (PP) [90] and model potential (MP) calculations [111, 112] model the response of the valence electrons with inclusion of effective potentials to treat the core electrons. An effective core potential is used similarly in the configuration interaction core potential (CICP) calculation of Müller, Flesch, and Meyer [113]. The CICP calculation of Mitroy and Bromley [97] utilizes a model that treats core excitation using effective oscillator strengths designed to reproduce the core polarizability. The multi-reference configuration interaction (MRCI) calculation of Partridge *et al.* [114] gives 71.2. They also calculated a CI-CV value of 70.3 (not listed in Table III), which is in good agreement with the similar calculation of 70.9 by Hamanou and Hibbert [52], but the average value of 74.37 from the CI-CV calculations by Moccia and Spizzo [115] is significantly larger. The coupled cluster double-excitation with contributions of single and triple excitations [CCD+ST (CCD)] model of Castro and Canuto [116] yields a value of 70.89, somewhat lower than the MRCI value and the fourth

TABLE II: A comparison of results for the principal resonance transition absorption oscillator strength for Mg. Abbreviations for methods are defined in the text. Where a calculation was carried out in the length gauge (LG) and the velocity gauge (VG), the simple average is listed and the LG and VG values are listed as a table footnote.

Method	f	Source	Ref. (Year)
MCDF-CV	1.709	Jönsson and Fischer	[51] (1997)
MCHF	1.717	Jönsson, Fischer, & Godefroid	[56] (1999)
MP	1.717	Victor and Laughlin	[63] (1973)
MCHF+BP	1.719	Fischer, Tachiev, & Irimia	[102] (2006)
RCI+Breit	1.722	Cheng *et al.*	[103] (2011)
CIDF-CP	1.72	Stanek, Glowacki, & Migdalek	[104] (1996)
CI+MBPT[a]	1.724	Savukov and Johnson	[105] (2002)
CI[b]	1.725	Mengali and Moccia	[106] (1996)
CI[c]	1.73	Nesbet and Jones	[107] (1977)
CI+MBPT[d]	1.73(2)	Derevianko and Porsev	[53] (2011)
CICP	1.732	Mitroy and Bromley	[97] (2003)
CI	1.735	Hamonou and Hibbert	[52] (2008)
CI[e]	1.737	Weiss	[62] (1967)
MCHF-CV	1.738	Zatsarinny *et al.*	[57] (2009)
MCHF[f]	1.747	Fischer	[54] (1975)
CI-frozen core	1.75	Chang and Tang	[65] (1990)
CI-CV[g]	1.755	Moccia and Spizzo	[76] (1988)
CI-frozen core	1.76	Saraph	[64] (1976)
NIST adopted[h]	1.8	Kelleher and Podobedova	[46] (2008)
Experiment[i]	1.83(3)	Morton	[45] (2003)

[a]Mean of LG and VG line strength with experimental transition energy from [46]

[b]Mean of LG 1.72 and VG 1.73

[c]Mean of LG 1.746 and VG 1.717

[d]Line strength with experimental transition energy from [46]

[e]Mean of LG 1.773 and VG 1.701

[f]Mean of LG 1.757 and VG 1.736

[g]Mean of LG 1.76 and VG 1.75

[h]Cited as Weiss, private communication. Using the CI value for the line strength from Weiss (1967) and the measured transition energy yields 1.77.

[i]Weighted average of ten experimental values as of 2003.

order many body perturbation theory [MBPT(4)] value of 71.7 calculated by Archibong and Thakkar [108], while the coupled cluster with single and double excitation-effective Hamiltonian (CCSD-EH) approach of Stanton [117] yields 72.2 using basis sets from Ref. [118], denoted WMR in the Table. The pseudo-natural orbital coupled electron pair approximation (PNO-CEPA) calculation of Reinsch and Meyer [101] is close to the CI+MBPT calculation of Porsev and Derevianko [47]. Two time-dependent density functional theory (TDDFT) calculations are included in Table III. Using time-dependent DFT with a self-interaction correction (TDDFT-SIC), Chu and Dalgarno [109] obtained 71.8 and using the symmetry adapted perturbation theory codes, SAPT(DFT), Patkowski *et al.* [119] obtained 73.27 for the polarizability. An extensive table of values for the polarizability of Mg resulting from various density functional theory functionals is given in Ref. [22]. The R-matrix calculation of Robb [120] is 75(5); the relatively large value results because core-valence correlation effects were not included [90]. Excluding the relatively large value from

TABLE III: The static electric dipole polarizability (in units of a_0^3) for Mg in the ground state. Abbreviations for methods are defined in the text.

Method	$\alpha(0)$	Source	Ref. (Year)
Experiment (cryogenic molecular beam)	59(15)	Ma *et al.*	[29] (2015)
QDT	69.54	Chernov *et al.*	[110] (2005)
PP	70.5	Maeder and Kutzelnigg	[90] (1979)
CICP	70.74(71)	Müller, Flesch, & Meyer	[113] (1984)
CCD+ST (CCD)	70.89	Castro and Canuto	[116] (1993)
CI	70.90	Hamanou and Hibbert	[52] (2008)
MRCI	71.2	Partridge *et al.*	[114] (1990)
CICP	71.35	Mitroy and Bromley	[97] (2003)
CI+MBPT	71.3(7)	Porsev and Derevianko	[47] (2006)
PNO-CEPA	71.32	Reinsch and Meyer	[101] (1976)
MBPT(4)	71.70	Archibong and Thakkar	[108] (1991)
TDDFT-SIC	71.8	Chu and Dalgarno	[109] (2004)
MP	72.0	Patil	[112] (2000)
MP	72.1	Victor and Slavsky	[111] (1974)
CCSD-EH (WMR)	72.2	Stanton	[117] (1994)
SAPT (DFT)	73.27	Patkowski *et al.*	[119] (2007)
CI-CV[a]	74.37	Moccia and Spizzo	[115] (1988)
Sum rule	74.4(2.7)	Reshetnikov *et al.*	[89] (2008)
R-matrix[b]	75(5)	Robb	[120] (1975)

[a]Mean of LG 74.7 and VG 74.03

[b]Does not include core valence according to Ref. [90]

Ref. [115], the CI, MRCI, CICP, and MBPT calculations fall in the range from 70.74 to 71.7. Reshetnikov *et al.* [89] use a semi-empirical method that utilizes a sum rule with constraints and error bars determined using measured the lifetime and excitation energies. Their value is 74.4(2.7), with the accuracy limited by the available input data. The recent experiment of Ma *et al.* [29] using a cryogenic molecular beam found a value of 59(15), which is not yet sufficiently accurate to test the calculations against.

Table IV presents a collection of van der Waals constant values from the literature and a significant range is apparent, though the CI+MBPT and CICP calculations, which include models of core electron excitations, are in good agreement. The value 620(5) from the model potential (MP) calculation of Santra, Christ, and Greene [121] is close close to the pseudopotential (PP) calculation of 618.4 from Maeder and Kutzelnigg [90], both of which include effective potentials to account for the presence of core electrons, but don't fully include their excitations. The MP calculation from Patil [112], however, is significantly larger, at 648. Three DFT calculations are listed in Table IV. Hult et al. [122] introduced a local dielectric function and cutoff on the interaction volume and obtained 615. In contrast, Chu and Dalgarno used time-dependent DFT with a self-interaction correction (TDDFT-SIC) and an empirical correction to obtain 626 with an estimated uncertainty of 1%. Patkoswki *et al.* [119] used the symmetry adapted perturbation theory codes, SAPT(DFT), and obtained 635. The calculation of C_6 by Stanton [117] used a quadrature and values of the dynamic polarizability at imaginary frequencies calculated using the CCSD-EH coupled cluster approach with the basis sets from [118]. The CI-CV calculations of Moccia and Spizzo [115] in the velocity gauge (VG) and in the length

TABLE IV: The dispersion constant (in units of $e^2 a_0^5$) for the Mg dimer from various references. Abbreviations for methods are defined in the text.

Method	C_6	Source	Ref. (Year)
DFT	615	Hult *at al.*	[122] (1999)
PP	618.4	Maeder and Kutzelnigg	[90] (1979)
MP[a]	620(5)	Santra, Christ, & Greene	[121] (2004)
TDDFT-SIC[b]	626(6)	Chu and Dalgarno	[109] (2004)
CI+MBPT	627(12)	Porsev and Derevianko	[47] (2006)
CICP	629.5	Mitroy and Bromley	[97] (2003)
MP	632.27	Victor and Slavsky	[111] (1974)
SAPT(DFT)	635	Patkowski *et al.*	[119] (2007)
CCSD-EH (WMR)	648	Stanton	[117] (1994)
MP	648	Patil	[112] (2000)
CI-CV (VG)	658.1	Moccia and Spizzo	[115] (1988)
CI-CV (LG)	670.9	Moccia and Spizzo	[115] (1988)
Empirical	683(35)	Stwalley	[88] (1971)
R-matrix	689(70)	Robb	[120] (1975)

[a]Does not include core contributions

[b]Listed in Table VII as "corrected," corresponding to an empirical rescaling.

gauge (LG) are substantially larger than the other listed calculations. Robb [120] estimated his R-matrix calculation to be accurate to 10 %. Stwalley [88] used an empirically constructed polarizability function to calculate C_6. The large value for C_6 corresponds to the choice of 1.82 for the principal oscillator strength. In Ref. [2] it was found that a 2% uncertainty in C_6 leads to an uncertainty of no more than 0.3 nm in the scattering length for $^{24}Mg_2$.

[1] E. Tiesinga, S. Kotochigova, and P. S. Julienne, Phys. Rev. A **65**, 042722 (2002).

[2] H. Knöckel, S. Rühmann, and E. Tiemann, J. Chem. Phys. **138**, 094303 (2013).

[3] H. Knöckel, S. Rühmann, and E. Tiemann, Eur. Phys. J. D **68**, 293 (2014).

[4] P. Soldan, P. S. Zuchowski, and J. M. Hutson, Discuss. Faraday Soc. **142**, 191 (2009).

[5] M. L. González-Martínez and J. M. Hutson, Phys. Rev. A **84**, 052706 (2011).

[6] V. P. A. Lonij, C. E. Klauss, W. F. Holmgren, and A. D. Cronin, J. Phys. Chem. A **115**, 7134 (2011).

[7] A. Vidal-Madjar, C. M. Huitson, V. Bourrier, J.-M. Désert, G. Ballester, A. Lecavelier des Etangs, D. K. Sing, D. Ehrenreich, R. Ferlet, G. Hébrard, and J. C. McConnell, Astron. Astroph. **560**, A54 (2013).

[8] V. Bourrier, A. Lecavelier des Etangs, and A. Vidal-Madjar, Astron. Astroph. **565**, A105 (2014).

[9] V. Bourrier, A. Lecavelier des Etangs, and A. Vidal-Madjar, Astron. Astroph. **573**, A11 (2015).

[10] A. Derevianko, S. Porsev, and J. Babb, At. Data Nucl. Data Tables **96**, 323 (2010).

[11] J. Jiang, J. Mitroy, Y. Cheng, and M. Bromley, At. Data Nucl. Data Tables **101**, 158 (2015).

[12] M. Y. Amusia, *Atomic Photoeffect* (Plenum, New York, 1990), trans. K. T. Taylor.

[13] M. Amusia, L. Chernysheva, and V. Yarzhemsky, *Handbook of Theoretical Atomic Physics Data for Photon Absorption, Electron Scattering, and Vacancies Decay* (Springer, Berlin, 2012).

[14] J. Berkowitz, *Atomic and Molecular Photoabsorption: Absolute Total Cross Sections* (Academic Press, San Diego, 2002).

[15] M. Masili and A. F. Starace, Phys. Rev. A **62**, 033403 (2000).

[16] T. Middelmann, S. Falke, C. Lisdat, and U. Sterr, Phys. Rev. Lett. **109**, 263004 (2012).

[17] J. A. Sherman, N. D. Lemke, N. Hinkley, M. Pizzocaro, R. W. Fox, A. D. Ludlow, and C. W. Oates, Phys. Rev. Lett. **108**, 153002 (2012).

[18] K. Beloy, J. A. Sherman, N. D. Lemke, N. Hinkley, C. W. Oates, and A. D. Ludlow, Phys. Rev. A **86**, 051404 (2012).

[19] J. E. Stalnaker, D. Budker, S. J. Freedman, J. S. Guzman, S. M. Rochester, and V. V. Yashchuk, Phys. Rev. A **73**, 043416 (2006).

[20] Z. W. Barber, J. E. Stalnaker, N. D. Lemke, N. Poli, C. W. Oates, T. M. Fortier, S. A. Diddams, L. Hollberg, C. W. Hoyt, A. V. Taichenachev, and V. I. Yudin, Phys. Rev. Lett. **100**, 103002 (2008).

[21] I. B. Khriplovich, *Parity Non-conservation in Atomic Phenomena* (Gordon and Breach, New York, 1991).

[22] R. Bast, A. Hesselmann, P. Sałek, T. Helgaker, and T. Saue, ChemPhysChem **9**, 445 (2008).

[23] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett. **102**, 073005 (2009).

[24] A. Tkatchenko, R. A. DiStasio, R. Car, and M. Scheffler, Phys. Rev. Lett. **108**, 236402 (2012).

[25] J. Tao, J. P. Perdew, and A. Ruzsinszky, Int. J. Mod. Phys. B **27**, 1330011 (2013).

[26] J. Toulouse, E. Rebolini, T. Gould, J. F. Dobson, P. Seal, and J. G. Angyan, J. Chem. Phys. **138**, 194106 (2013).

[27] D. Goebel and U. Hohm, Phys. Rev. A **52**, 3691 (1995).

[28] G. S. Sarkisov, I. L. Beigman, V. P. Shevelko, and K. W. Struve, Phys. Rev. A **73**, 042501 (2006).

[29] L. Ma, J. Indergaard, B. Zhang, I. Larkin, R. Moro, and W. A. de Heer, Phys. Rev. A **91**, 010501 (2015).

[30] P. Schwerdtfeger, in *Atoms, Molecules, and Clusters in Electric Fields*, edited by G. Maroulis (Imperial College Press, London, 2006), Chap. 1, p. 1.

[31] A. J. Thakkar and C. Lupinetti, in *Atoms, Molecules, and Clusters in Electric Fields*, edited by G. Maroulis (Imperial College Press, London, 2006), Chap. 14, pp. 505–530.

[32] J. Mitroy, M. S. Safronova, and C. W. Clark, J. Phys. B **43**, 202001 (2010).

[33] S. Dimopoulos and A. A. Geraci, Phys. Rev. D **68**, 124021 (2003).

[34] D. M. Harber, J. M. Obrecht, J. M. McGuirk, and E. A. Cornell, Phys. Rev. A **72**, 033610 (2005).

[35] B. Murphy and L. V. Hau, Phys. Rev. Lett. **102**, 033003 (2009).

[36] A. Derevianko, B. Obreshkov, and V. A. Dzuba, Phys. Rev. Lett. **103**, 133201 (2009).

[37] V. A. Dzuba and A. Derevianko, J. Phys. B: At. Mol. Opt. Phys. **43**, 074011 (2010).

[38] B. Arora, H. Kaur, and B. K. Sahoo, J. Phys. B **47**, 155002 (2014).

[39] U. D. Jentschura, G. Łach, M. De Kieviet, and K. Pachucki, Phys. Rev. Lett. **114**, 043001 (2015).

[40] J. Tao and J. P. Perdew, J. Chem. Phys. **141**, 141101 (2014).

[41] P. Kharchenko, J. F. Babb, and A. Dalgarno, Phys. Rev. A **55**, 3566 (1997).

[42] F. A. van Abeelen and B. J. Verhaar, Phys. Rev. A **59**, 578 (1999).

[43] S. Knoop, T. Schuster, R. Scelle, A. Trautmann, J. Appmeier, M. K. Oberthaler, E. Tiesinga, and E. Tiemann, Phys. Rev. A **83**, 042704 (2011).

[44] A. Derevianko, W. R. Johnson, M. S. Safronova, and J. F. Babb, Phys. Rev. Lett. **82**, 3589 (1999).

[45] D. C. Morton, Astrophys. J., Suppl. Ser. **149**, 205 (2003).

[46] D. E. Kelleher and L. I. Podobedova, J. Phys. Chem. Ref. Data **37**, 267 (2008).

[47] S. G. Porsev and A. Derevianko, Zh. Eksp. Teor. Fiz. **129**, 227 (2006), [JETP **102**, 195 (2006)].

[48] C. J. Mitchell, J. Phys. B **8**, 25 (1975).

[49] C. Mendoza and C. J. Zeippen, Astron. Astroph. **179**, 339 (1987).

[50] D. Ray and P. K. Mukherjee, J. Phys. B **22**, 2103 (1989).

[51] P. Jönsson and C. F. Fischer, J. Phys. B **30**, 5861 (1997).

[52] L. Hamonou and A. Hibbert, J. Phys. B **41**, 245004 (2008).

[53] A. Derevianko and S. G. Porsev, *Adv. At. Molec. Opt. Phys.*, edited by E. Arimondo, P. R. Berman, and C. C. Lin

(Academic Press, Amsterdam, 2011), Vol. 60, Chap. 9, pp. 415 – 459.

[54] C. F. Fischer, Can. J. Phys. **53**, 338 (1975).

[55] G. A. Victor, R. F. Stewart, and C. Laughlin, Ap. J., Suppl. **31**, 237 (1976).

[56] P. Jönsson, C. F. Fischer, and M. R. Godefroid, J. Phys. B **32**, 1233 (1999).

[57] O. Zatsarinny, K. Bartschat, S. Gedeon, V. Gedeon, V. Lazur, and E. Nagy, Phys. Rev. A **79**, 052709 (2009).

[58] S. G. Porsev, M. G. Kozlov, Y. G. Rakhlina, and A. Derevianko, Phys. Rev. A **64**, 012508 (2001).

[59] W. L. Wiese, J. R. Fuhr, and B. M. Miles, *Atomic Transition Probabilities, Vol. II: Sodium through Calcium, NSRDS-NBS Vol. 22* (US GPO, Washington, D.C., 1969).

[60] A. Lurio, Phys. Rev. **136**, A376 (1964).

[61] W. W. Smith and A. Gallagher, Phys. Rev. **145**, 26 (1966).

[62] A. W. Weiss, J. Chem. Phys. **47**, 3573 (1967).

[63] G. Victor and C. Laughlin, Nucl. Instrum. Methods **110**, 189 (1973).

[64] H. E. Saraph, J. Phys. B **9**, 2379 (1976).

[65] T. N. Chang and X. Tang, J. Quant. Spectrosc. Radiat. Transfer **43**, 207 (1990).

[66] R. W. Ditchburn and G. V. Marr, Proc. Phys. Soc., London, Sect. A **66**, 655 (1953).

[67] A. Burgess and M. J. Seaton, Mon. Not. R. Astron. Soc. **120**, 121 (1960).

[68] G. N. Bates and P. L. Altick, J. Phys. B **6**, 653 (1973).

[69] W. H. Parkinson, E. M. Reeves, and F. S. Tomkins, J. Phys. B **9**, 157 (1976).

[70] P. C. Deshmukh and S. T. Manson, Phys. Rev. A **28**, 209 (1983).

[71] J. M. Preses, C. E. Burkhardt, W. P. Garver, and J. J. Leventhal, Phys. Rev. A **29**, 985 (1984).

[72] V. Radojević and W. R. Johnson, Phys. Rev. A **31**, 2991 (1985).

[73] J. Yeh and I. Lindau, At. Dat. Nucl. Dat. Tables **32**, 1 (1985).

[74] C. F. Fischer and H. P. Saha, Can. J. Phys. **65**, 772 (1987).

[75] C. Mendoza and C. J. Zeippen, Astron. Astroph. **179**, 346 (1987).

[76] R. Moccia and P. Spizzo, J. Phys. B **21**, 1133 (1988).

[77] Z. Altun, Phys. Rev. A **40**, 4968 (1989).

[78] D. A. Verner, D. G. Yakovlev, I. M. Band, and M. B. Trzhaskovskaya, At. Dat. Nucl. Dat. Tables **55**, 233 (1993).

[79] H.-C. Chi and K.-N. Huang, Phys. Rev. A **50**, 392 (1994).

[80] H. S. Fung and T. S. Yih, Nucl. Phys. A **684**, 696C (2001).

[81] D.-S. Kim and S. S. Tayal, J. Phys. B: At. Mol. Opt. Phys. **33**, 3235 (2000).

[82] R. Wehlitz, D. Lukić, and P. N. Juranić, J. Phys. B **40**, 2385 (2007).

[83] A. Hausmann, B. Kämmerling, H. Kossmann, and V. Schmidt, Phys. Rev. Lett. **61**, 2669 (1988).

[84] G. Wang, J. Wan, and X. Zhou, J. Phys. B **43**, 035001 (2010).

[85] M. S. Pindzola, C. P. Ballance, S. A. Abdel-Naby, F. Robicheaux, G. S. J. Armstrong, and J. Colgan, J. Phys. B **46**, 035201 (2013).

[86] T. G. Lee, C. P. Ballance, S. A. Abdel-Naby, J. L. King, T. W. Gorczyca, and M. S. Pindzola, J. Phys. B **48**, 065201 (2015).

[87] B. L. Henke, P. Lee, T. J. Tanaka, R. L. Shimabukuro, and B. K. Fujikawa, At. Dat. Nucl. Dat. Tables **27**, 1 (1982).

[88] W. C. Stwalley, J. Chem. Phys. **54**, 4517 (1971).

[89] N. Reshetnikov, L. J. Curtis, M. S. Brown, and R. E. Irving, Phys. Scr. **77**, 015301 (2008).

[90] F. Maeder and W. Kutzelnigg, Chem. Phys. **42**, 95 (1979).

[91] M. Kutzner, V. Maycock, J. Thorarinson, E. Pannwitz, and J. A. Robertson, Phys. Rev. A **66**, 042715 (2002).

[92] M. F. Hasoğlu, S. A. Abdel-Naby, E. Gatuzz, J. García, T. R. Kallman, C. Mendoza, and T. W. Gorczyca, Astrophys. J., Suppl. Ser. **214**, 8 (2014).

[93] M. Banna, A. Slaughter, R. Mathews, R. Key, and S. Ballina, Chem. Phys. Lett. **92**, 122 (1982).

[94] G. Nasreen, S. T. Manson, and P. C. Deshmukh, Phys. Rev. A **40**, 6091 (1989).

[95] V. G. Pal'chikov and V. D. Ovsiannikov, Quantum Electronics **34**, 412 (2004).

[96] V. D. Ovsyannikov, V. G. Pal'chikov, H. Katori, and M. Takamoto, Quantum Electron. **36**, 3 (2006).

[97] J. Mitroy and M. W. J. Bromley, Phys. Rev. A **68**, 052714 (2003).

[98] S. G. Porsev and A. Derevianko, Phys. Rev. A **65**, 020701 (2002).

[99] C. Froese Fischer, P. Jönsson, and M. Godefroid, Phys. Rev. A **57**, 1753 (1998).

[100] V. P. A. Lonij, C. E. Klauss, W. F. Holmgren, and A. D. Cronin, Phys. Rev. Lett. **105**, 233202 (2010).

[101] E.-A. Reinsch and W. Meyer, Phys. Rev. A **14**, 915 (1976).

[102] C. Froese Fischer, G. Tachiev, and A. Irimia, At. Dat. Nucl. Dat. Tables **92**, 607 (2006).

[103] C. Cheng, X. Gao, B. Qing, X.-L. Zhang, and J.-M. Li, Chin. Phys. B **20**, 033103 (2011).

[104] M. Stanek, L. Glowacki, and J. Migdalek, J. Phys. B **29**, 2985 (1996).

[105] I. M. Savukov and W. R. Johnson, Phys. Rev. A **65**, 042503 (2002).

[106] S. Mengali and R. Moccia, J. Phys. B **29**, 1613 (1996).

[107] R. K. Nesbet and H. W. Jones, Phys. Rev. A **16**, 1161 (1977).

[108] E. F. Archibong and A. J. Thakkar, Phys. Rev. A **44**, 5478 (1991).

[109] X. Chu and A. Dalgarno, J. Chem. Phys. **121**, 4083 (2004).

[110] V. E. Chernov, D. L. Dorofeev, I. Y. Kretinin, and B. A. Zon, Phys. Rev. A **71**, 022505 (2005).

[111] G. A. Victor and D. B. Slavsky, J. Chem. Phys. **61**, 3484 (1974).

[112] S. Patil, Eur. Phys. J. D **10**, 341 (2000).

[113] W. Müller, J. Flesch, and W. Meyer, J. Chem. Phys. **80**, 3297 (1984).

[114] H. Partridge, C. W. Bauschlicher Jr., L. G. M. Pettersson, A. D. McLean, B. Liu, M. Yoshimine, and A. Komornicki, J. Chem. Phys. **92**, 5377 (1990).

[115] R. Moccia and P. Spizzo, J. Phys. B **21**, 1145 (1988).

[116] M. A. Castro and S. Canuto, Phys. Lett. A **176**, 105 (1993).

[117] J. F. Stanton, Phys. Rev. A **49**, 1698 (1994).

[118] P. Widmark, B. Joakim Persson, and B. Roos, Theo. Chim. ACTA **79**, 419 (1991).

[119] K. Patkowski, R. Podeszwa, and K. Szalewicz, J. Phys. Chem. A **111**, 12822 (2007).

[120] W. D. Robb, Chem. Phys. Lett. **34**, 479 (1975).

[121] R. Santra, K. V. Christ, and C. H. Greene, Phys. Rev. A **69**, 042510 (2004).

[122] E. Hult, H. Rydberg, B. I. Lundqvist, and D. C. Langreth, Phys. Rev. B **59**, 4708 (1999).